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MEMORANDUM

SUBJECT: Review: Lower Passaic River Bioaccumulation Model

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TO: Ray Basso
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Attached are my comments on the Lower Passaic River Bioaccumulation model prepared by Windward Environmental, LLC for the LPR Cooperating Parties Group (CPG)

cc:
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Dale Hoff
Edward Garland
Paul Paquin
Kevin Farley

Model spreadsheets examined:
20131218 bioaccumulation model template - Steady State.xlsm
20131218 bioaccumulation model template - Dynamic.xlsm
20131218 dynamic bioaccumulation model input template.xlsx

General Modeling Code:
The steady-state spreadsheet model developed by the CPG contains the code for the Arnot and Gobas (2004) food web bioaccumulation model, and it appears to be coded correctly, i.e., the computation of the residues in the organisms appears to be correct.

Dietary Absorption Efficiencies:
For benthic species of benthic deposit feeder, benthic detritivore, small benthic ominivore, large benthic omnivore, and blue crab, the CPG model dietary lipid and NLOM (non-lipid organic matter) absorption efficiencies are 15% in both the steady-state and dynamic spreadsheets. These values are substantially less than those suggested by Arnot and Gobas of 75% for lipid and NLOM dietary absorption efficiencies for aquatic invertebrates. Windward provides no scientific information supporting the use of such low absorption efficiencies in the present model. Previously, Windward applied the Arnot and Gobas (2004) model at the Lower Duwamish Waterway Superfund site and via Monte Carlo analyses for two different calibration data sets, arrived at the following absorption efficiencies:

Lipid and NLOM Absorption Efficiencies: Taken from "Table D.5-4. Best-fit parameter sets for Calibration 1 and 2" of the Lower Duwamish Waterway Remedial Investigation, Remedial Investigation Report, Appendix D. Food Web Model. November 5, 2007.			
Species	Absorption Efficiencies	Calibration 1	Calibration 2
Benthic Invertebrates	Lipid	30%	79%
	NLOM	56%	61%
Slender Crab	Lipid	75%	66%
	NLOM	76%	54%
Dungeness Crab	Lipid	71%	36%
	NLOM	56%	68%

The above derived dietary adsorption efficiencies for lipid and NLOM are 2 to 5 fold larger than the values selected for the CPG Passaic River bioaccumulation model. Even given the rather limited data sets for the Lower Duwamish site and the variability that often occurs with field measurements, their derived dietary absorption efficiencies are strongly supportive of the 75% dietary absorption efficiencies recommended by Arnot and Gobas (2004). EPA was also provided a report on a San Francisco Bay PCB Food Web Model (Gobas and Wilcockson (2003)) by Windward Environmental supporting their use of the Arnot and Gobas model for the Passaic River. In that application the aquatic invertebrates had lipid and NLOM absorption efficiencies of 75% (i.e., the recommended value of Gobas and Arnot).

Lowering the dietary absorption efficiencies for lipid and NLOM from 75% to 15% will decrease the predicted residues for the benthic invertebrate species, and for species preying upon them. Determining the exact level of decrease would require running of the model with 75% and 15% absorption efficiencies while leaving the other input parameters unchanged.

With the Arnot and Gobas model, dietary absorption efficiencies for lipid and NLOM of 72% are recommended for zooplankton. In the CPG Passaic River formulation of the model, dietary absorption efficiencies for lipid and NLOM of 55% were used for zooplankton, and no justification is provided for using values not recommended by Arnot and Gobas (2004).

The impact of using the lower dietary absorption efficiencies for lipid and NLOM is that higher contaminant concentrations in the sediment will be required to predict a given tissue residue. The corollary of this, as indicated above, is that for a given sediment concentration, using lower dietary absorption efficiencies for lipid and NLOM will decrease the predicted residues for benthic invertebrate species, and for species preying upon them.

Biotransformation Rate (k_m) of 2,3,7,8-TCDD

Biotransformation of 2,3,7,8-TCDD by fish has been reported in the literature. The database of fish biotransformation rates for organic chemicals by Arnot et al. (2007) provides estimates of whole body fish biotransformation rates (k_m; units 1/days) for 10 g fish at 15°C based upon laboratory data for carp (log k_m of -1.72, -1.84, -2.12), fathead minnow (-2.05, -2.14), guppy (-2.08), and rainbow trout (-1.62). The median and average of the log k_m values are -2.05 and -1.94, respectively, and taking the antilog, k_m values for a 10 g fish at 15°C are 0.00891 and 0.0115 (1/days). Biotransformation rates scale according to size (weight of the organism) and temperature (°C) to the general equation Arnot et al. (2007):

(1)

where W_{10} = 10 gram fish
T_{15} = Temperature of 15°C
W_i = Weight of fish "i" in grams
T_i = Environmental temperature in °C for fish "i"
$k_{m,10g\ 15°C}$ = Whole body biotransformation rate for a 10 g fish at 15°C
$k_{m,i}$ = Whole body transformation rate for fish "i"of weight (W_i) at temperature (T_i)

In the CPG Passaic River steady-state and dynamic models, a biotransformation rate of 0.0136 (1/day) for fish was used except for American eel that had a k_m of 0.040 (1/day). The weights of the fish in the CPG Passaic River model ranged from 3.1 to 3170 grams. No documentation was provided on the source of the biotransformation rate constant for fish.

Below are estimates of biotransformation rates appropriately scaled for both weight and temperature using the median and average k_m values from the Arnot et al. (2007) database. The biotransformation rates for fish and blue crab from the CPG steady-state spreadsheet model are provided as well.

CPG Lower Passiac River Bioaccumulation Model: Weights and metabolic rate constants for fish and blue crab											
	Species	FFF (8)	SFF (9)	BC (10)	SMB (11)	LMB (12)	WP (13)	WC (14)	CC (15)	CAR (16)	AE (17)
Weight	kg	0.011	0.0031	0.17	0.23	0.29	0.097	0.918	0.82	3.17	0.27
Metabolic rate constant	K_M (1/d)	0.0136	0.0136	0.0136	0.0136	0.0136	0.0136	0.0136	0.0136	0.0136	0.0400

Metabolic rate constants (k_m; units 1/days) for 10 g Fish at 15°C from the Arnot et al. (2007) Database for 2,3,7,8-TCDD										
								average	median	n
log k_m	-1.72	-1.84	-2.12	-2.05	-2.14	-2.08	-1.62	-1.94	-2.05	7
							k_m	0.0115	0.00891	

Estimated metabolic rate constants for fish and blue crab (k_m; units 1/days) for the Lower Passaic River using the median and average k_m values after adjustment for organism weight and to a ecosystem temperature of 13.8°C											
	Species	FFF (8)	SFF (9)	BC (10)	SMB (11)	LMB (12)	WP (13)	WC (14)	CC (15)	CAR (16)	AE (17)
median k_m		0.00860	0.0118	0.00435	0.00401	0.00379	0.00499	0.00284	0.00293	0.00209	0.00386
Ratio: Estimated k_m to CPG bioaccumulation model input parameter											
		63%	87%	32%	29%	28%	37%	21%	22%	15%	10%
average k_m		0.0111	0.0153	0.00563	0.00518	0.00489	0.00645	0.00368	0.00378	0.00270	0.00499
Ratio: Estimated k_m to CPG bioaccumulation model input parameter											
		82%	112%	41%	38%	36%	47%	27%	28%	20%	12%

Species Code	
FFF (8)	filter feeding fish (e.g., menhaden)
SFF (9)	small forage fish (e.g., mummichog)
BC (10)	blue crab
MB (11)	smallmouth bass
LMB (12)	largemouth bass
WP (13)	white perch
WC (14)	white catfish
CC (15)	channel catfish
CAR (16)	carp
AE (17)	american eel

For fish with weights greater than 10 grams (or 0.01 kg), the biotransformation rates estimated for Passaic River fish using the Arnot et al. (2007) database and methodology are substantially lower than the constant value of 0.0136 (1/d) used in the CPG Passaic River bioaccumulation model, e.g., 3 to 10 fold lower.

The CPG model also has biotransformation rates for the benthic deposit feeder, benthic detritivore, small benthic ominivore, and large benthic omnivore of 0.023 (1/day). No documentation supporting the biotransformation rate is provided.

It is well known that benthic invertebrates have substantially less metabolic ability to biotransform organic contaminants in comparison to fish. I'm unaware of any published biotransformation rates for aquatic invertebrates for 2,3,7,8-TCDD. Further, it is generally accepted that PCBs are rarely if at all biotransformed by aquatic invertebrates. Modeling study by Morrison et al. (1999) for TCDD in the Lake Ontario food web suggests that benthic invertebrates have biotransformation rates that are, at a minimum, 2 orders lower than fish. A conservative assumption, for modeling purposes, would be to replace the 0.023 (1/day) values with 0.0.

The net result of having biotransformation rates that are too large is that higher contaminant concentrations in the sediment will be required to predict a given residue. Similarly, for a given sediment contaminant concentration, if the biotransformation rates are assumed to be too large the results would be to lower the predicted tissue residue.

Dynamic Model
The model is set up with all organisms having no growth. By this, I mean, for each modeling time step, the weight of the organism at the start of the time step is the same. Ecological conditions such as age-class structure and organisms growing over time are not incorporated into the model.

The time step appears to be one month.

I'm unsure of the correctness of the CPG numerical method for computing the concentrations over time. For zooplankton (#3 species), this is the equation:

The differential equation for zooplankton is:

The equation in the spreadsheet is not a solution based upon the slope nor is it a numerical integration method like Gears, Euler, or Runga-Kutta. Their computation needs to be verified before moving forwards with the outputs from the dynamic model.

Summary Comments:
The CPG Lower Passaic River bioaccumulation model uses, what I believe, are unsupportable, based upon the current literature, input values for the dietary absorption efficiencies for lipid and NLOM (non-lipid organic matter) for benthic invertebrates, and for biotransformation rates for 2,3,7,8-TCDD in fish and benthic invertebrates. Use of the model with the appropriate values will increase the total accumulation of the chemical across the entire food web, i.e., from sediments to all organisms. With the appropriate values, the current differences existing between Region 2's the BSAF approach and CPG's Lower Passaic River bioaccumulation model will decrease.

References

Arnot, J. A., & Gobas, F. A. (2004). A food web bioaccumulation model for organic chemicals in aquatic ecosystems. *Environmental Toxicology and Chemistry,* 23(10), 2343-2355.

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Morrison, H. A., Whittle, D. M., Metcalfe, C. D., & Niimi, A. J. (1999). Application of a food web bioaccumulation model for the prediction of polychlorinated biphenyl, dioxin, and furan congener concentrations in Lake Ontario aquatic biota. *Canadian Journal of Fisheries and Aquatic Sciences*, 56(8), 1389-1400.